From:	PETERSON Jenn L
To:	Eric Blischke/R10/USEPA/US@EPA; Burt Shephard/R10/USEPA/US@EPA
Subject:	FW: Water Equation
Date:	06/26/2008 08:48 PM
Attachments:	BSF calcs.doc

Burt and Eric,

I asked Bruce to briefly help out in answering the water question. From his response (see Case 1 versus 2), it you can see the implications for using the LWG water equation. The key questions now would be what data are they using to calculate DOC (see Bruce's comment) and is it sufficient, and are they limiting the water data used in the model to the XAD data (e.g. no total water at all)? Also, we would have to be aware that the LWG model would be extremely sensitive to the selected Kow.

-Jennifer

-----Original Message-----
From: HOPE Bruce
Sent: Thursday, June 26, 2008 2:20 PM
To: PETERSON Jenn L
Cc: POULSEN Mike; ANDERSON Jim M
Subject: RE: Water Equation

Jennifer,

Well, the LWG text you faxed me isn't a model of clarity.

They don't use POC at all; DOC is implicit in the "Cwd,o" term in equations 1 and 2, page 3.

POC is missing from equation 6 on page 5 because they are assuming, as did Morrison (1997), that all of the POC-associated chemical was filtered out and thus there is no need to consider it. The 0.08 constant is that recommended by Burkhard (2000) and should be OK.

As the attached example illustrates, which method you use (POC/DOC & total or DOC & filtered) makes a big difference in the estimate of the freely available fraction.

But, even though it may be to their advantage to do so, I don't think what they're doing is wrong per se. But it's an estimate which is critically dependent on both KOW and DOC - I assume they've got plentiful, accurate measurements of DOC?

I have no idea what the statement about "... no overlying water information..." means.

Hope this helps a bit ... have to get back to fine particulate issues.

Bruce

> -----Original Message-----
> **From:** PETERSON Jenn L
> **Sent:** Wednesday, June 25, 2008 2:51 PM
> **To:** HOPE Bruce

Subject: Water Equation

Bruce,

Here is the Morrison 1997 paper - look at Equation 15. The modification here is the basis for their change. I am also faxing you pages 3-5 from the Round 2 Report. The model assumptions and set up are on pages 3 and 4. There are no terms for POC and DOC (or their associated proportionality constants). Look at Equation 6 on Page 5 for the water equation - they are using a factor of 0.08, but POC is absent. Also, notice they state "because the model was modified to use XAD sample information, which directly estimates freely dissolved water concentration, no overlying water information was needed".

-Jennifer